Object-Oriented Molecular Simulation Programs
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The aim of this project is to develop an object-oriented framework for molecular simulation programs using Monte Carlo techniques. The resulting framework will make it easy to develop, and rapidly prototype, condensed-matter simulation codes for a variety of molecular models.

The focus will be on models composed of non-spherical building blocks which interact in a variety of ways, involving both continuous and discontinuous functions of their separation and relative orientation. The software framework should make it possible to apply a wide range of Monte Carlo trial moves, including multi-particle, cluster-based, and configurational-biased moves for polymers, as well as extracting a range of physical properties and averages from the simulations.

Molecular simulation codes are typically cpu-intensive and it will be important to retain the high performance characteristics of existing programs written in the traditional way, in Fortran, as much as possible. Ideally the programming language will be Fortran 2003, but I am willing to discuss the possibilities of using C++, or developing a Python framework with an interface to another language to handle the cpu-intensive parts.

For examples of this approach in the relevant area, see the following references.

References


